

# Approximate analytic solution for electronic wave functions and energies in coupled quantum wells

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A formalism is developed which results in simple analytic expressions for the electron energy splittings and the wave functions in coupled quantum well structures of the type employed in new laser and transistor configurations. The limits of validity of the formalism are explored.

The ability to fabricate single and multiple quantum well devices has given rise to numerous new optical and electronic devices as well as to new physical phenomena.<sup>1-3</sup>

An increasing amount of recent attention has been directed to structures employing more than one quantum well with interwell spacings and barriers sufficiently small so that significant amounts of (tunneling) interaction takes place.<sup>4,5</sup> We will refer to such structures as Coupled Quantum Wells (CQW). Two important issues which arise here are those of the effect of coupling on the (quantized) energies and on the electron localization. These affect directly the performance of optical (lasers) and electronic (e.g., field-effect transistor) devices.

An approximate expression for the energy splitting based on an exact solution of the two (identical) well Schrödinger equations was obtained in Ref. 4 while numerical solution of the effect of well asymmetry on the electron distribution was considered in Ref. 5.

In the work reported below we will present a formalism which leads to simple analytic expressions for the eigenfunctions and eigenenergies of the coupled square quantum wells. An additional feature of the theory is that it yields convenient expressions for the effect of intentional and unintentional deviations from structure symmetry on the eigenenergies and the electron localization. It also suggests how the electronic or optical properties of such devices might be controlled by means of an external field.

The potential energy function  $V(x)$  of our model problem is plotted in Fig. 1(a). The height asymmetry  $\phi$  and the well width difference ( $t_2 - t_1$ ), both exaggerated in the figure, are small and represent the slight intentional or accidental departures from that of an ideal structure.

Drawing on a formalism employed successfully to describe optical directional couplers,<sup>6</sup> we express an eigenstate  $\psi(x)$  of an electron in the potential  $V(x)$  of Fig. 1(b) as a linear combination of well orbitals (LCWO)  $\psi_{1,2}(x)$  of the two separate wells in the limit of infinite separation ( $a \rightarrow \infty$ ), i.e.,

$$\psi(x) = a\psi_1(x) + b\psi_2(x), \quad (1)$$

where the Schrödinger equations obeyed by  $\psi_{1,2}(x)$  are the single-well equations

$$H_{1,2}\psi_{1,2} = E_{1,2}\psi_{1,2}, \quad (2)$$

$$H_{1,2} = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_{1,2}(x), \quad (3a)$$

and  $m^*$  is the carrier effective mass. The single-well potential energy functions  $V_{1,2}(x)$  are shown in Fig. 2(b).

We note that the CQW potential  $V(x)$  can be expressed as

$$V(x) = V_1(x) + V_2(x) - V_0; \quad (3b)$$

the Schrödinger equation now takes the form

$$\left( -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_1(x) + V_2(x) - V_0 \right) (a\psi_1 + b\psi_2) = \tilde{E} [a\psi_1 + b\psi_2], \quad (4)$$

since  $\psi_1(x)$  and  $\psi_2(x)$  are presumed known [they involve a solution of the standard one-dimensional square-well Schrödinger Eq. (2)]. The solution of Eq. (4) reduces to a determination of the eigenfunction coefficients  $a$  and  $b$  and eigenenergies  $\tilde{E}$ .

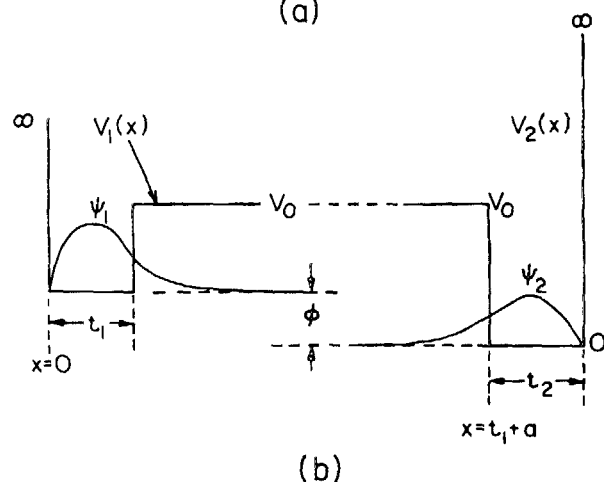
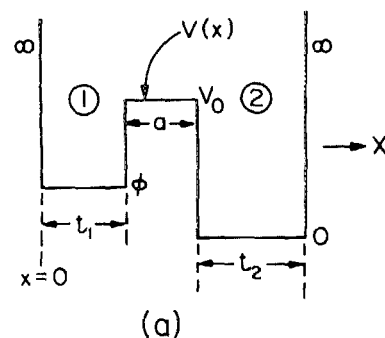


FIG. 1. (a) Energy  $V(x)$  of a double well structure; (b) the individual potential energies  $V_1(x)$  and  $V_2(x)$  of the single-well structures whose eigenfunctions are combined to obtain those of the double-well structure.

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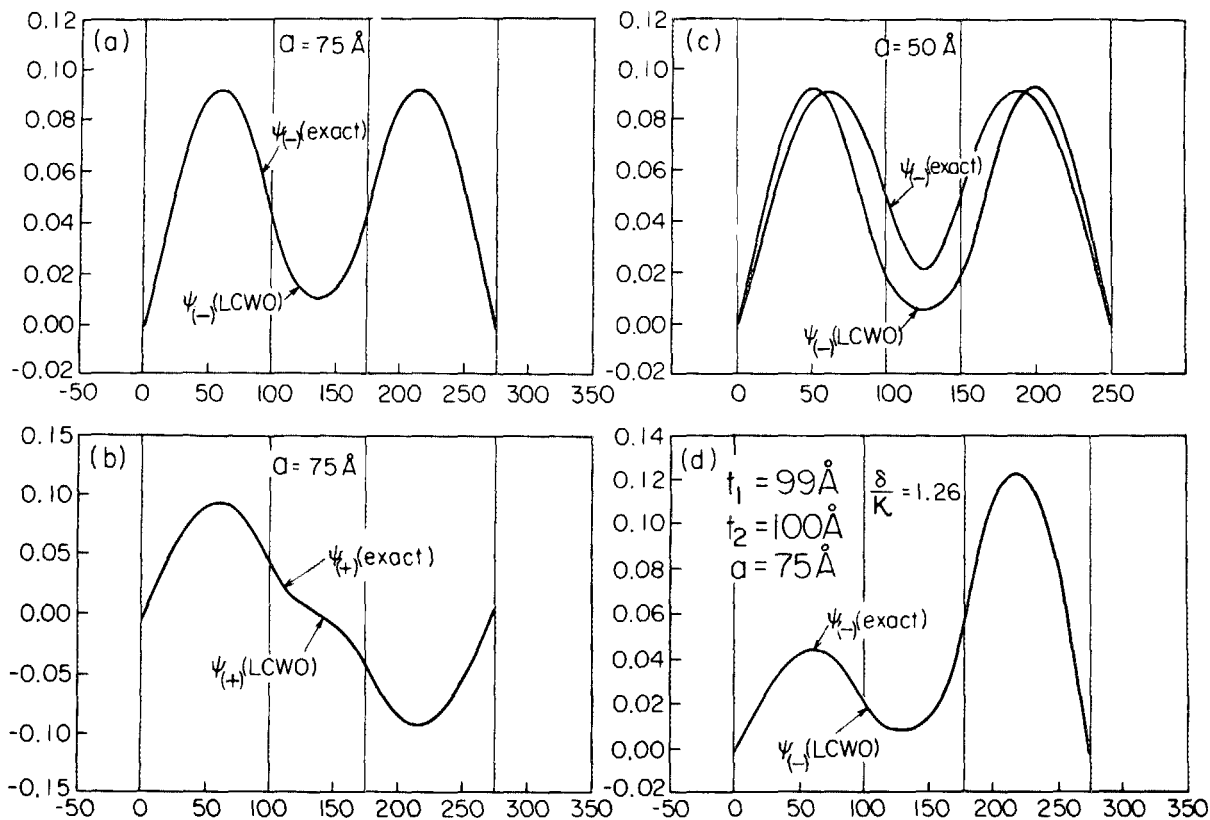


FIG. 2. The exact and LCWO wave functions for different barrier widths:  $V_0 = 0.15$  eV,  $m^* = 0.1m$ ,  $\phi_0$ , and  $t_1 = t_2 = 100$  Å except in 2(d) where  $t_1 = 99$  Å,  $t_2 = 100$  Å.

Equation (4) simplifies to

$$a[(E_1 - \tilde{E}) + (V_2(x) - V_0)]\psi_1 + b[(E_2 - \tilde{E}) + (V_1(x) - V_0)]\psi_2 = 0,$$

where  $E_1$  and  $E_2$  are the (known) single-well eigenenergies.

Next we multiply 5 by  $\psi_1^*$  and integrate from  $-\infty$  to  $\infty$  and repeat the procedure using  $\psi_2^*$ . The respective results are

$$\begin{aligned} a[(E_1 - \tilde{E}) + \langle 1|V_2 - V_0|1 \rangle] + b[(E_2 - \tilde{E})\langle 1|2 \rangle + \langle 1|V_1 - V_0|2 \rangle] &= 0, \\ a[(E_1 - \tilde{E})\langle 2|1 \rangle] + [\langle 2|V_2 - V_0|1 \rangle] + b[(E_2 - \tilde{E}) + \langle 2|V_1 - V_0|2 \rangle] &= 0. \end{aligned} \quad (6)$$

It is convenient to introduce new energy parameters

$$\delta \equiv \frac{E_1 - E_2}{2}, \quad E = \frac{E_1 + E_2}{2}, \quad \epsilon = E - \tilde{E}, \quad (7)$$

which transforms Eq. (6) to

$$\begin{vmatrix} (\epsilon + \delta) + \langle 1|V_2 - V_0|1 \rangle & (\epsilon - \delta)\langle 1|2 \rangle + \langle 1|V_1 - V_0|2 \rangle \\ (\epsilon + \delta)\langle 2|1 \rangle + \langle 2|V_2 - V_0|1 \rangle & (\epsilon - \delta) + \langle 2|V_1 - V_0|2 \rangle \end{vmatrix} \begin{vmatrix} a \\ b \end{vmatrix} = 0. \quad (8)$$

The explicit determination of all the matrix elements involved in Eq. (8) has been carried out by using the normalized single-well solutions  $\psi_1(x)$  and  $\psi_2(x)$ . The general results are rather complicated. In the case of  $V_0 \gg E_{1,2}$  and of weak coupling ( $Ka \gg 1$ ) considered here, we have for the symmetric case

$$\begin{aligned} \langle 1|2 \rangle &\approx 8 \left( \frac{E}{V_0} \right) \frac{1}{Kt} e^{-\kappa a}, \\ \langle 1|V_2 - V_0|1 \rangle &\approx \langle 2|V_1 - V_0|2 \rangle \sim \frac{E}{Kt} e^{-2\kappa a}, \\ \langle 1|V_1 - V_2|2 \rangle &\approx \langle 2|V_2 - V_0|1 \rangle \approx 4 \frac{E}{Kt} e^{-\kappa a}, \end{aligned} \quad (9)$$

$$K = \sqrt{\frac{2m^*}{\hbar^2}(V_0 - E)}.$$

In all cases of interest here  $\exp(-Ka) \ll 1$ ,  $\delta, \epsilon \ll E$  so that to a high degree of accuracy we may replace Eq. (8) with

$$\begin{vmatrix} \epsilon + \delta & \kappa_1 \\ \kappa_2 & \epsilon - \delta \end{vmatrix} \begin{vmatrix} a \\ b \end{vmatrix} = 0, \quad (10)$$

whose determinantal equation gives

$$\epsilon(\pm) = \pm \sqrt{\delta^2 + \kappa_1 \kappa_2}, \quad (11)$$

where

$$\begin{aligned} \kappa_1 &\equiv \langle 1|V_1(x) - V_0|2 \rangle, \\ \kappa_2 &\equiv \langle 2|V_2(x) - V_0|1 \rangle, \end{aligned} \quad (12)$$

are the coupling constants. The eigenenergies are thus given by

$$\begin{aligned}\tilde{E}^{(+)} &= E + \epsilon^{(+)} = \frac{1}{2}(E_1 + E_2) + \sqrt{\delta^2 + \kappa_1 \kappa_2}, \\ \tilde{E}^{(-)} &= E + \epsilon^{(-)} = \frac{1}{2}(E_1 + E_2) - \sqrt{\delta^2 + \kappa_1 \kappa_2},\end{aligned}\quad (13)$$

and the corresponding normalized eigenfunctions obtained after substituting  $\epsilon^{(+)}$  and  $\epsilon^{(-)}$ , one at a time, in Eq. (10) to solve for  $a/b$ , are

$$\begin{aligned}(\text{Energy } \tilde{E}^{(+)}) \quad \psi_{\text{odd}} &= \frac{(\sqrt{\delta^2 + \kappa^2} - \delta)}{[\kappa^2 + (\sqrt{\delta^2 + \kappa^2} - \delta)^2]^{1/2}} \psi_1 \\ &\quad - \frac{\kappa_2}{[\kappa^2 + (\sqrt{\delta^2 + \kappa^2} - \delta)^2]^{1/2}} \psi_2,\end{aligned}\quad (14)$$

$$\begin{aligned}(\text{Energy } \tilde{E}^{(-)}) \quad \psi_{\text{odd}} &= \frac{\kappa_1}{[\kappa^2 + (\sqrt{\delta^2 + \kappa^2} - \delta)^2]^{1/2}} \psi_1 \\ &\quad + \frac{(\sqrt{\delta^2 + \kappa^2} - \delta)}{[\kappa^2 + (\sqrt{\delta^2 + \kappa^2} - \delta)^2]^{1/2}} \psi_2,\end{aligned}\quad (15)$$

where  $\kappa^2 \equiv \kappa_1 \kappa_2$ .

In the symmetric case,  $\delta = 0$ ,  $\kappa_1 = \kappa_2$ , and  $a^{(+)} = a^{(-)} = b^{(+)} = -b^{(-)} = 1/\sqrt{2}$  as expected, i.e., the eigenfunctions possess even or odd parity. In the weak coupling limit which we are considering the coupling constants  $\kappa_1$  and  $\kappa_2$  are given by

$$\kappa_1 = -(V_0 - \phi) \left( \frac{4}{t_1 t_2} \right)^{1/2} \frac{k_1 k_2}{K_1 K_2} \frac{K_1 + K_2}{K_1^2} e^{-\kappa_2 a}, \quad (16)$$

$$\kappa_2 = -V_0 \left( \frac{4}{t_1 t_2} \right)^{1/2} \frac{k_1 k_2}{K_1 K_2} \frac{K_1 + K_2}{K_2^2} e^{-\kappa_1 a}, \quad (17)$$

$$k_1 = \sqrt{\frac{2m^*(E_1 - \phi)}{\hbar^2}}, \quad K_1 = \sqrt{\frac{2m^*(V_0 - E_1)}{\hbar^2}},$$

$$k_2 = \sqrt{\frac{2m^*E_2}{\hbar^2}}, \quad K_2 = \sqrt{\frac{2m^*(V_0 - E_2)}{\hbar^2}}. \quad (18)$$

In the case of small asymmetry considered here  $\phi \ll V_0$  and  $K_1 \approx K_2$ ,  $E_1 \approx E_2$ ,  $k_1 \approx k_2$ , the expression for the coupling constant simplifies to

$$\kappa_1 \approx \kappa_2 = \kappa = 4 \left( \frac{V_0 - E}{V_0} \right) \frac{E}{1 + Kt} e^{-\kappa a}. \quad (19)$$

An important parameter is the energy splitting between the two states of the TCQW structure. It is given, according to Eq. (13) by

$$\Delta E \equiv \tilde{E}^{(+)} - \tilde{E}^{(-)} = 2\sqrt{\delta^2 + \kappa_1 \kappa_2}, \quad (20)$$

which in the symmetric case ( $\delta = 0$ ) reduces to

$$\Delta E = 2\kappa = 8 \frac{(V_0 - E)}{V_0} \frac{E}{1 + Kt} e^{-\kappa a}. \quad (21)$$

The last result agrees with that obtained by Kroemer and Okamoto<sup>5</sup> from a solution of the boundary value problem of a symmetric two coupled quantum well structures. A comparison with an *exact* numerical solution of the eigenvalue problem of Eq. (4) is shown in Table I. We find that in our example the error between the exact energy splitting and the LCWO result of Eq. (21) is less than 2% for barriers exceeding 75 Å in width. The condition for validity of the LCWO result is  $\exp(-\kappa a) \ll 1$  (i.e., small tunneling probability). We can thus extend the range of validity of the LCWO to even narrower barriers by increasing the barrier height ( $V_0$ ), or the well width ( $t$ ) or using an electron with a larger  $m^*$  (our example uses a conservative value of  $m^* = 0.1 m$ ).

The basic physical parameter determining the electron localization is the ratio  $\delta/\kappa$ . When  $\delta \ll \kappa$  the wave functions according to Eq. (14) are distributed essentially equally between the wells while for  $\delta \gg \kappa$  we have from Eq. (14) that

$$\begin{aligned}\psi_{\text{odd}} &\rightarrow \frac{\kappa/2\delta}{\left(1 + \frac{\kappa^2}{8\delta^2}\right)} \psi_1 - \frac{1}{\left(1 + \frac{\kappa^2}{8\delta^2}\right)} \psi_2 \\ &\approx \frac{\kappa}{2\delta} \psi_1 - \psi_2 \approx \psi_2,\end{aligned}\quad (22)$$

while

$$\begin{aligned}\psi_{\text{even}} &\rightarrow \frac{1}{\left(1 + \frac{\kappa^2}{8\delta^2}\right)} \psi_1 + \frac{\kappa/2\delta}{\left(1 + \frac{\kappa^2}{8\delta^2}\right)} \psi_2 \\ &\approx \psi_1 + \frac{\kappa}{2\delta} \psi_2 \approx \psi_1,\end{aligned}\quad (23)$$

and the wave functions become highly localized in one of the two wells. We can thus control the degree of localization of an electron in a TCQW structure by controlling the ratio  $\delta/\kappa$ . A comparison between the LCWO wave functions Eqs. (14), (15) and the exact functions obtained by a numerical solution of the Schrödinger equation is shown in Fig. 2. In Figs. 2(a) and 2(b) we show, respectively, the symmetric and antisymmetric wave functions in a symmetric well with a barrier width of 75 Å. The exact and approximate (LCWO) eigenenergies differ by less than 0.6% so that in this figure

TABLE I. A comparison of the exact value of the energy and that calculated from the LCWO result Eq. (21).

$a(\text{Å})$	150	100	75	50	25
$E$ (eV)		0.0276892	same	same	same
$\exp(-\kappa a)$	$\sim 0$	0.0035	0.014	0.059	0.25
$\Delta E_{\text{exact}}$ (eV)	$\sim 0$	$9.376 \times 10^{-5}$	$3.860 \times 10^{-4}$	$1.578 \times 10^{-3}$	$6.174 \times 10^{-3}$
$\Delta E_{\text{LCWO}} - \Delta E_{\text{exact}}$	$\sim 0$	0.55	1.85	10.6	64
$\frac{\Delta E_{\text{LCWO}}}{\Delta E_{\text{exact}}}$ (percent)					

the corresponding eigenfunctions appear identical. An appreciable deviation of the approximate solution from the exact solution appears when the barrier width is reduced to 50 Å as can be seen in Fig. 2(c). We note that, according to Table I, the error in the energy splitting in this case is only  $\sim 10\%$ . A comparison of the exact and approximate wave functions in an asymmetric structure is shown in Fig. 2(d). The discrepancy between the exact and the LCWO functions is not visible in this drawing. We note also that the very strong localization, 89% of  $|\psi|^2$  in the right well, is brought about by a mere 1 Å ( $= 1\%$ ) difference between the well widths. The mismatch parameter  $\delta$  is given in the weak-coupling,  $[\exp(-ka) \ll 1]$  near-symmetric case by

$$\delta \approx \frac{\phi}{2} - \frac{\hbar^2 \pi^2}{m^* t^3} (t_1 - t_2),$$

$$t \equiv \frac{1}{2} (t_1 + t_2). \quad (24)$$

We can thus compensate for a geometric mismatch when ( $t_1 \neq t_2$ ) by using an asymmetric potential field,  $\phi \neq 0$  so that a symmetric ( $\delta = 0$ ) quantum well structure does not consist necessarily of identical wells. The control of  $\phi$  can be accomplished by an applied bias field across the structure. Applica-

tions to field-controlled field-effect transistors and lasers suggest themselves.

In summary, we have presented an analytic approach (LCWO) for solving the Schrödinger equation of coupled quantum well structures. Two parameters,  $\kappa$  and  $\delta$ , characterize the electronic energy splitting and the electron localization. The LCWO formalism should apply equally well to the case of coupled wells which are not square, where the exact solution will prove impractical, as well as to the multi-quantum-well case.

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